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HOT H_2 AND INTERSTELLAR SHOCKS

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ABSTRACT

The rotational excitation of H_2 molecules by interstellar shock waves is calculated. Level populations integrated through a shock in a cloud of density of 10 cm^{-3} have nearly exponential distributions, with effective rotational temperatures $T_r = 15\,V^{1.5}$ ° K, where V is the shock velocity in km s^{-1}. Ortho-para conversion is effective for high shock velocities, but not for low ones, so that the degree of alternation of intensities of rotational lines in the Lyman absorption band should be correlated with V, and therefore with T_r. The results are compared with observations of H_2 rotational levels made by the *Copernicus* satellite.

Subject headings: excitation and ionization — molecules — shock waves

I. INTRODUCTION

Observation of interstellar shock waves has so far been prevented by blending problems in 21-cm observations, and by low detection sensitivity for the infrared emission lines expected theoretically (Field *et al.* 1968). However, data on H_2 molecules from the *Copernicus* satellite (Spitzer *et al.* 1973) have provided information which may prove the existence of interstellar shocks, as considerable excitation of the higher rotational levels $J = 4$, 5, and 6 in the ground electronic and vibrational state of the molecule is observed. The observed column densities N_J correspond to rotational temperatures greater than 200° K, considerably higher than the temperatures near 100° K deduced both from the lower rotational levels in H_2 and from the 21-cm absorption-line studies. We propose that the higher rotational excitations reflect conditions in shock waves which are propagating through the absorbing interstellar clouds, and which incorporate only a small fraction of the total cloud mass. The much cooler preshock and postshock gas determines the excitation of the lower rotational levels and does not contribute to the observed column densities for the higher J levels. The source of the shock waves may be expanding H II regions around the early-type stars, propagating outward at 5–10 km s^{-1} in the later phases of expansion. Alternatively, the shocks could be caused by cloud-cloud collisions along the line of sight.

II. SHOCK STRUCTURE AND ROTATIONAL EXCITATION OF H_2

We assume that the region of the shock where translational, rotational, and fine-structure degrees of freedom are excited is infinitesimally thick, and we treat only the cooling region in detail, as in our earlier work (Field *et al.* 1968; Aannestad 1973*b*). The assumption of instantaneous equilibrium for the rotational levels of H_2 is not accurate when H_2/H exceeds 0.1, because then the cooling occurs on the same time scale as the excitation of the rotational levels. Neglect of H_2–H_2 collisions compared with H–H_2 collisions may also become important for $H_2/H > 0.1$. Pending completion of the more detailed calculations needed for $H_2/H > 0.1$, we present here the results for $H_2/H = 0.1$. The problem of scaling the results to compare with the observations ($H_2/H = 0.04$–1.0) is discussed in § IV.

The presence of a transverse magnetic field $B = 3$ microgauss is taken into account as outlined by Field *et al.* (1968), and complete coupling between the field and the neutral gas is assumed. As shown by Mullan (1971), for low ion densities this becomes increasingly inaccurate for small shock velocities (~ 5 km s^{-1}). However, with the higher ion densities provided by nonthermal ionization ($n_i/n_H \simeq 4 \times 10^{-3}$), the assumption is still valid. Throughout the shock the electron density is essentially frozen to its preshock value because of the long recombination time. The ionization rate is taken to be 4×10^{-16} s^{-1}.

The state of the preshock gas is chosen to agree roughly with the observational data from *Copernicus*. The temperature is 80° K, reflecting an ortho-para ratio of unity (Spitzer *et al.* 1973). The preshock n_H is 10 cm^{-3}, typical of interstellar clouds (Spitzer 1968). The element abundances in the gas phase are decreased by factors which are average values from figure 1 of Morton *et al.* (1973): 0.2, 0.8, 0.2, 0.25, 0.16, and 0.1, for C, N, O, Si, Mg, and Fe, respectively. The underabundance of Si and heavier elements in the gas is attributed to their presence in the cores of interstellar dust particles (Field 1973), and the depletion of C, N, and O is assumed to be due to mantle formation (Aannestad 1973*a*). For a core radius of 0.05 μ, a core density of 2.5 g cm^{-3}, and a mantle density of 1.5 g cm^{-3}, the adopted depletion implies a dust/gas ratio $n_g/n_H = 4 \times 10^{-12}$ and a grain radius of 0.1 μ.

The grain-gas interaction is treated as described by Aannestad (1973*b*), neglecting the influence of the magnetic field on the motion of the grains. The magnetic field probably increases sputtering of the mantle in some respects and decreases it in others, so it is not known which way neglect of the magnetic effect on the grains biases the results. However, since sputtering is important only for $V \geqslant 10$ km s^{-1}, most of the results reported here should not be significantly affected.

The preshock ortho-para ratio is taken equal to unity, and ortho-para conversion via H_2 (para) $+$ H $(k) \rightleftarrows H_2$ (ortho) $+$ H is included with a rate constant $k = 2.4 \times 10^{-11}\, T^{1/6}\, e^{-3900/T}$ cm^3 s^{-1} (Schofield 1967). The H_2 photodissociation rate is 1×10^{-14} s^{-1}, accounting for the effects of self-shielding according to Hollenbach *et al.* (1971). Thermal dissociation of H_2 is also included, but is usually negligible for the range of shock velocities considered here.

The shocked gas in general cools down to temperatures substantially lower than the preshock values. However, the thermal state of this cool gas is quite uncertain because of the onset of molecular cooling and rapid depletion of cooling elements onto dust grains. Thus we arbitrarily terminate the calculations when the temperature reaches the preshock temperature of 80° K. This does not affect the predicted column densities for the higher J levels which are of concern here.

III. RESULTS

The column density of H_2 molecules in the Jth level (N_J), measured through the postshock region and normal to the shock front, is given in figure 1 for the preshock conditions described in § II and for shock velocities of 4, 6, 9, and 13 km s^{-1}. (Results are given in terms of $N_J{}^* = N_J/g_J$.) In spite of the complexity of the processes occurring in the postshock region, the curves of $N_J{}^*$ versus E have the approximate form exp $(-E_J/kT_r)$, where T_r is an effective rotational excitation temperature. To within 10 percent, T_r is a constant independent of the particular ortho or para levels considered. Study of the local densities n_J of excited molecules at various points behind the shock front shows that contributions to n_J for the higher J levels are predominantly from the immediate postshock region, where the temperature is high enough to excite those levels. At each point, statistical equilibrium demands that

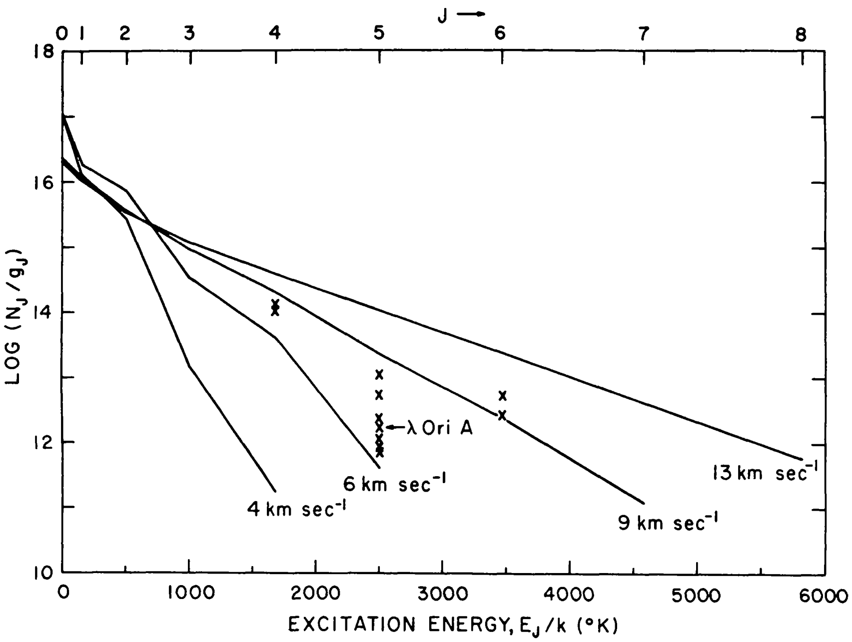

FIG. 1.—Predicted column densities per unit statistical weight, $N_J^* = N_J/g_J$, integrated through shock and normal to it, for four shock velocities and for $H_2/H = 0.1$. The observations (*crosses*) from Spitzer *et al.* (1973) refer to somewhat different values of H_2/H (ranging from 0.4 to 1.0). No corrections have been introduced for this or for angles between the line of sight and the normal to the shock. The star λ Ori A is believed to have an expanding H II region around it (see text).

$$\frac{n_J}{n_{J-2}} = \frac{\exp(-\Delta E_J/kT)}{1 + A/C}, \qquad (1)$$

where T is the local kinetic temperature and A and C are the downward radiative and collisional rates, respectively (Field *et al.* 1968). Equation (1) shows that the exponential dependence is modified by the factor A/C in the integration to obtain column densities. As A/C is an increasing function of J, this causes the population ratios to drop increasingly below the exponential based upon the temperature T. Remarkably, the result is another exponential, corresponding to a lower temperature, $T_r \leqslant T$. In table 1 we list the values of the immediate postshock temperature and T_r (deduced from N_J^* for the $J = 4$ and 6 levels) for various shock velocities. Empirically, we find that $T_r = 15V^{1.5}$ ° K.

The other qualitative feature that emerges from figure 1 is a varying degree of

TABLE 1

SHOCK PROPERTIES

Shock Velocity V (km s^{-1})	Immediate Postshock Temperature (° K)	Effective Rotational Temperature T_r (° K)	Ortho-Para Parameter $\langle R \rangle$
4	245	120	0.3
6	696	222	0.4
9	1890	406	0.9
13	4354	662	1.0

ortho-para alternation of intensities. To characterize this, we calculated the equilibrium values $N_J{}^*{}_{,\mathrm{eq}}$ for $J = 3$ and 5 from the column density N_4 and T_r as deduced from the ratio N_5/N_3. The ratios $R_J = N_J{}^*/N_J{}^*{}_{,\mathrm{eq}}$ for $J = 3$ and 5 measure the deviations from ortho-para equilibrium ($R_J = 1$). The mean, $\langle R \rangle$, of R_3 and R_5 is given in table 1. For $V = 13$ km s^{-1}, $\langle R \rangle$ is near unity, reflecting the fact that at the high postshock temperatures involved (4350° K) ortho-para conversion is so rapid that an equilibrium is approached which depends only upon E_J. For lower velocities, postshock temperatures are progressively lower, and ortho-para conversion is progressively inhibited and so the ortho-para ratio is frozen at the initial value of unity, rather than at the equilibrium value of 3.

IV. COMPARISON WITH OBSERVATIONS

In figure 1 we have plotted the populations of certain rotational levels as reported for 11 stars (excepting δ Ori) by Spitzer *et al.* (1973). These data refer to values of H_2/H ranging from 0.04 to 1, with a mean value of 0.22, compared with the theoretically assumed 0.10. Theory and observations are not directly comparable, because the latter often refer to somewhat larger values of H_2/H and also because the line of sight may encounter the shock front at an angle, increasing the column density. Unfortunately, we cannot readily extrapolate our results for $H_2/H = 0.1$ to larger values since the problem is nonlinear. Probably a typical observational point should be moved downward in figure 1 by about half an order of magnitude in order to compare with the theory. Most of the observations are then consistent with shock velocities between about 6 and 9 km s^{-1}. Such shocks can be produced by cloud-cloud collisions and by expanding H II regions, such as those expected around the target stars themselves (§ 1).

It is known (Wade 1958) that the H II region of λ Ori A is surrounded by a shell of neutral gas, which according to 21-cm observations is moving radially outward at 8 km s^{-1}. If the excited H_2 observed in this star is due to a shock driven by the H II at this velocity, the line of sight would be perpendicular to the shock front and the projection factor would be unity. Since H_2/H is 0.06 for this star, the observed value of $N_5{}^*$ should be increased somewhat to compare with theory in figure 1. It is interesting that the corrected observational point indicates that $V \simeq 7$ km s^{-1}.

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